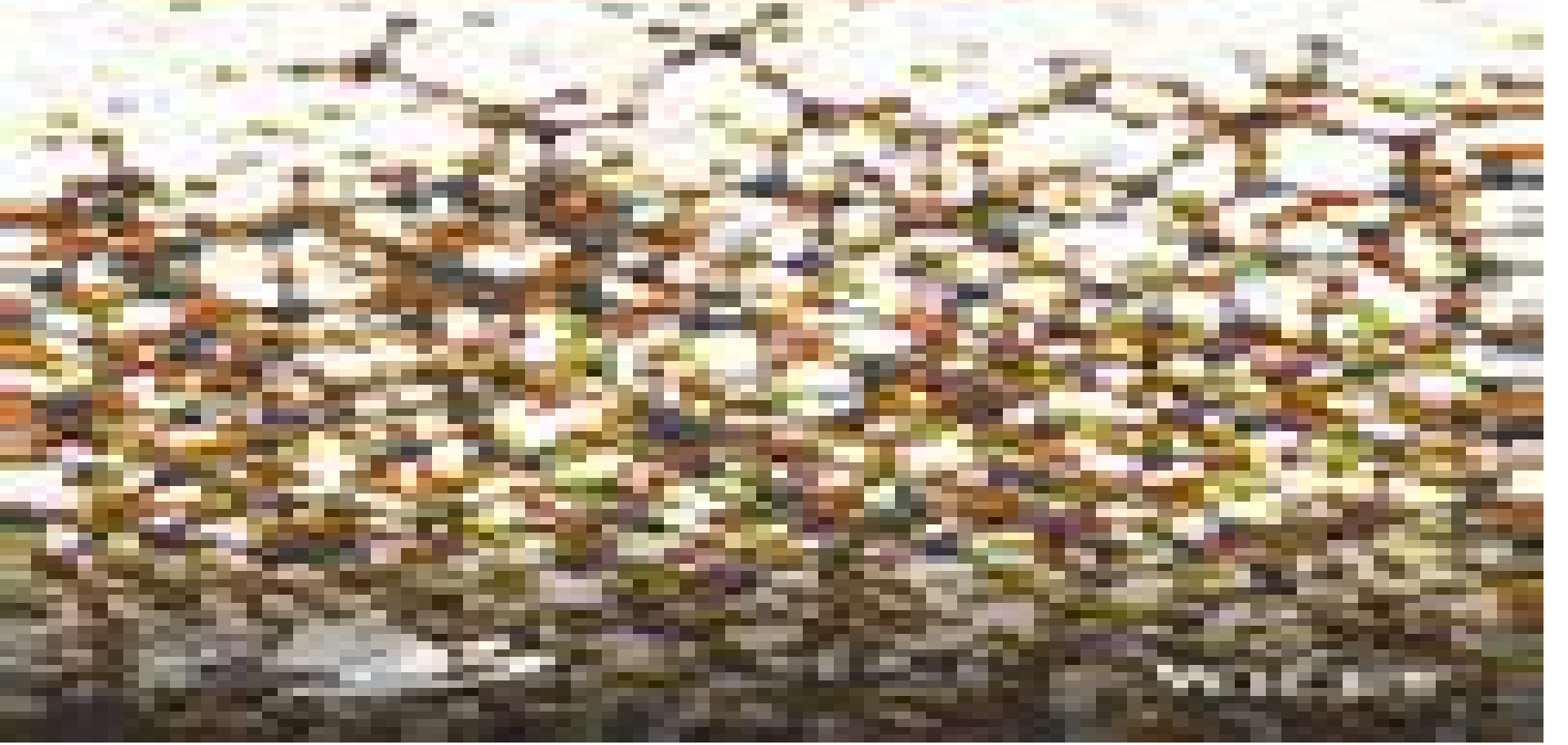
Atomistic Simulations of Glasses



Online Atomistic Computer Simulations Inorganic Glasses

Soumya Swayamjyoti

Online Atomistic Computer Simulations Inorganic Glasses:

Atomistic Simulations of Glasses Jincheng Du,Alastair N. Cormack,2022-03-29 A complete reference to computer simulations of inorganic glass materials In Atomistic Simulations of Glasses Fundamentals and Applications a team of distinguished researchers and active practitioners delivers a comprehensive review of the fundamentals and practical applications of atomistic simulations of inorganic glasses The book offers concise discussions of classical first principles Monte Carlo and other simulation methods together with structural analysis techniques and property calculation methods for the models of glass generated from these atomistic simulations before moving on to practical examples of the application of atomistic simulations in the research of several glass systems The authors describe simulations of silica silicate aluminosilicate borosilicate phosphate halide and oxyhalide glasses with up to date information and explore the challenges faced by researchers when dealing with these systems Both classical and ab initio methods are examined and comparison with experimental structural and property data provided Simulations of glass surfaces and surface water reactions are also covered Atomistic Simulations of Glasses includes multiple case studies and addresses a variety of applications of simulation from elucidating the structure and properties of glasses for optical electronic architecture applications to high technology fields such as flat panel displays nuclear waste disposal and biomedicine The book also includes A thorough introduction to the fundamentals of atomistic simulations including classical ab initio Reverse Monte Carlo simulation and topological constraint theory methods Important ingredients for simulations such as interatomic potential development structural analysis methods and property calculations are covered Comprehensive explorations of the applications of atomistic simulations in glass research including the history of atomistic simulations of glasses Practical discussions of rare earth and transition metal containing glasses as well as halide and oxyhalide glasses In depth examinations of glass surfaces and silicate glass water interactions Perfect for glass ceramic and materials scientists and engineers as well as physical inorganic and computational chemists Atomistic Simulations of Glasses Fundamentals and Applications is also an ideal resource for condensed matter and solid state physicists mechanical and civil engineers and those working with bioactive glasses Graduate students postdocs senior undergraduate students and others who intend to enter the field of simulations of glasses would also find the book highly valuable **Frontiers in Materials: Rising Stars** Nicola Maria Pugno,Diego Cazorla-Amoros,Jie-Sheng Chen,Guang-Ling Song,Sheikh A Akbar,Lothar Wondraczek,Alessandro Pegoretti,Seung-Bok Choi,John L. Provis,Jinn P. Chu,Krisztian Kordas,Liming Dai,2020-04-17 The Frontiers in Materials Editorial Office team are delighted to present the inaugural Frontiers in Materials Rising Stars article collection showcasing the high quality work of internationally recognized researchers in the early stages of their independent careers All Rising Star researchers featured within this collection were individually nominated by the Journal s Chief Editors in recognition of their potential to influence the future directions in their respective fields The work presented here highlights the diversity of research performed across

the entire breadth of the materials science and engineering field and presents advances in theory experiment and methodology with applications to compelling problems This Editorial features the corresponding author s of each paper published within this important collection ordered by section alphabetically highlighting them as the great researchers of the future The Frontiers in Materials Editorial Office team would like to thank each researcher who contributed their work to this collection We would also like to personally thank our Chief Editors for their exemplary leadership of this article collection their strong support and passion for this important community driven collection has ensured its success and global impact Laurent Mathey PhD Journal Development Manager *Geological Melts* Daniel R. Neuville,Grant S. Henderson,Donald B. Dingwell,2022-07-04 Volume 87 of Reviews in Mineralogy and Geochemistry covers fundamental aspects of the nature of silicate melts and the implications for the systems in which they participate both technological and natural The contents of this volume may perhaps best be summarized as structure properties dynamics The volume contains syntheses of short and medium range order structure property relationships and computation based simulations of melt structure It continues with analyses of the properties mechanical diffusive thermochemical redox nucleation rheological of melts The dynamic behavior of melts in magmatic and volcanic systems is then treated in the context of their behavior in magma mixing strain localization frictional melting magmatic fragmentation and hot sintering Finally the non magmatic extraterrestrial and prehistoric roles of melt and glass are presented in their respective contexts **Guide to Programs** National Science Foundation (U.S.),1997 Guide to Programs National Science Foundation (U.S.),1998 Compilation of funding opportunities for research and education in science mathematics and engineering **Chemical Abstracts** ,1991 Ceramic Abstracts ,1991 **Government Reports Announcements & Index** ,1996 Guide to Programs : Fiscal Year ... National Science Foundation,1998 Heterogeneities in Metallic Glasses: Atomistic Computer Simulations on the Structure and Mechanical Properties of Copper-zirconium Alloys and Composites Tobias Brink,2017 Science Citation Index ,1995 Vols for 1964 have guides and journal lists *Applications of Atomistic Simulation to Radioactive and Hazardous Waste Glass Formulation Development* ,1995 Glass formulation development depends on an understanding of the effects of glass composition on its processibility and product quality Such compositional effects on properties in turn depend on the microscopic structure of the glass Historically compositional effects on macroscopic properties have been explored empirically e g by measuring viscosity at various glass compositions The relationship of composition to structure has been studied by microstructural experimental methods More recently computer simulation has proved a fruitful complement to these more traditional methods of study By simulating atomic interaction over a period of time using the molecular dynamics method a direct picture of the glass structure and dynamics is obtained which can verify existing concepts as well as permit measurement of quantities inaccessible to experiment Atomistic simulation can be of particular benefit in the development of waste glasses As vitrification is being considered for an increasing variety of waste streams process and product models are

needed to formulate compositions for an extremely wide variety of elemental species and composition ranges The demand for process and product models which can predict over such a diverse composition space requires mechanistic understanding of glass behavior atomistic simulation is ideally suited for providing this understanding Moreover while simulation cannot completely eliminate the need for treatability studies it can play a role in minimizing the experimentation on and therefore contact handling of such materials This paper briefly reviews the molecular dynamics method which is the primary atomistic simulation tool for studying glass structure We then summarize the current state of glass simulation emphasizing areas of importance for waste glass process product modeling At SRS glass process and product models have been formulated in terms of glass structural concepts **Computer Simulation and Atomistic Modelling of Materials** Institute of Physics. Atomic Collisions in Solids Group,1993 *Fundamentals of Inorganic Glasses* Arun K. Varshneya,John C. Mauro,2019-05-09 Fundamentals of Inorganic Glasses Third Edition is a comprehensive reference on the field of glass science and engineering that covers numerous significant advances This new edition includes the most recent advances in glass physics and chemistry also discussing groundbreaking applications of glassy materials It is suitable for upper level glass science courses and professional glass scientists and engineers at industrial and government labs Fundamental concepts chapter ending problem sets an emphasis on key ideas and timely notes on suggested readings are all included The book provides the breadth required of a comprehensive reference offering coverage of the composition structure and properties of inorganic glasses Clearly develops fundamental concepts and the basics of glass science and glass chemistry Provides a comprehensive discussion of the composition structure and properties of inorganic glasses Features a discussion of the emerging applications of glass including applications in energy environment pharmaceuticals and more Concludes chapters with problem sets and suggested readings to facilitate self study Atomistic-simulations of Silicate Glasses Seung Ho Hahn,2020 Silicate based glasses are one of the most versatile materials in terms of technological perspective with a wide range of industrial applications In most cases glass products are exposed to various aqueous environments either humid air or liquid water and subject to physical contact with foreign objects which leads to deterioration of chemical and mechanical properties of glass surfaces Therefore understanding their interactions with adsorbed interfacial water molecules is critical as it can provide physical insights needed for rational design of more durable glasses Experimental characterization approaches have been applied to tackle difficult problems associated with the complex nature of glass surfaces but they are often limited by the time scale resolution As a result they have failed to offer important structural characteristics and chemical reaction mechanisms under dynamic processes happening at the glass surface To complement the challenges that experimental endeavors are encountering this dissertation aims to provide a comprehensive understanding of water interactions of silicate glass surfaces using atomistic scale simulations techniques In particular ReaxFF reactive force field based molecular dynamics MD simulations are employed to study two distinct surface phenomena i surface water reaction

and ii surface mechanochemical wear process These studies represent the surface damage process of silicate glass in the absence and presence of mechanical actions respectively The first part of this dissertation describes the water interactions of a silicate glass with readily leachable alkali sodium ions In this study highly complex surface chemistry including proton water exchange with the sodium ions formation of relatively long living sodium hydroxide ionic complexes at the glass surface and eventual dissolution of those ion pairs into the water phase are described Also surface mapping of water binding energy to the glass surface is evaluated at different stages of the glass water reaction which would be relevant to assess the chemical durability of the glass materials based on the glass network topology After the transport behavior and glass water reaction mechanism at the surface has been identified the mechanochemical wear process of sodium silicate glass rubbed with amorphous silica in the absence and presence of interfacial water molecules is covered in the second part of this dissertation The effect of water molecules on the shear induced chemical reaction at the sliding interface was investigated and the dependence of wear on the number of interfacial water molecules in ReaxFF MD simulations was found to be qualitatively in reasonable agreement with the experimental data The large scale atomistic simulation approaches with ReaxFF reactive force field presented in this dissertation alleviates the limitations of DFT calculations and experiments providing new and meaningful insights on the chemical dynamics associated within the glass water interface Optical Constants of Inorganic Glasses Andrei M. Efimov,2020-01-29 This book is devoted to the problem of the frequency dispersion of optical constants of inorganic glasses It is the only source providing a comprehensive discussion of this topic on a unified physical and analytical basis Optical Constants of Inorganic Glasses presents thorough descriptions of the underlying physical phenomena analytical models for the optical constants dispersion and detailed information on the optical constants and related optical characteristics of glasses The broad scope of the book includes such topics as general relationships for the response of a solid to the effect of an electromagnetic field and specific features of optical spectrum formation for a glass and the resulting constants The text details methods for reconstructing the spectra of optical constants from raw experimental spectra of glasses and provides data on the spectra of optical constants in the IR and VUV ranges and on the IR band parameters for inorganic glasses It includes factors responsible for the behavior of the refractive index dispersion of glasses in the transparency range The reference fully details the opportunities provided by the recent version of dispersion analysis for glasses based on the specific analytical model for the complex dielectric constant Until now this information was only available in Russian journals A large quantity of never before published data on numerical values of optical constants in the medium and far IR and of IR band frequencies and intensities is given for a wide variety of inorganic glasses For vitreous silica data on the optical constants are also given for the broad wavelength range in the VUV Optical Constants of Inorganic Glasses provides the only comprehensive review of available dispersion formulas and methods for interpolating and extrapolating the refractive indices of glasses in the transparency range The volume is a valuable resource for researchers

practitioners in the fields of glass technology Atomistic Simulation Techniques for Modelling Inorganic/organic Interface and Flotation Collector Design Tarun Kumar Kundu,2004 **Atomistic Simulations to Study Metallic Glasses: a Microscopic Investigation of Local Structural Excitations** Soumya Swayamjyoti,2016 **Atomistic Computational Approaches in Molecular Models and Inorganic Crystallization** Tesia Danielle Janicki,2022 Atomistic simulations provide a necessary lens through which to characterize nanoscale phenomena This dissertation begins with a description of molecular models and the development of aninteratomic potential for benzene which incorporates atomic level anisotropy This model was made possible for bulk benzene systems through the implementation of a software plugin for the OpenMM simulation package which enables custom force expressions with atomic level anisotropy This initial discourse on force field development summarizes the types of interatomic potentials used in simulations and avenues for improved accuracy This knowledge of fundamental force field development is transferrable to developing approaches in modeling inorganic crystallization Solid phase epitaxy SPE is a crystal growth technique which employs low temperature annealing conditions to exact kinetic control over the final grown structure In this dissertation classical simulations are used to rigorously define the mechanism of epitaxial growth in strontium titanate over patterned substrates Modeling SPE is challenging from a simulation perspective because long timescales at experimental growth temperature exceed computational feasibility The enhanced sampling method metadynamics is presented here as a viable alternative for probing crystallization mechanisms in super cooled and viscous systems for which diffusion is limited Gaining mechanistic information from metadynamics is dependent on the goodness of reaction coordinate Here an XRD based coordinate is used to distinguish not only between the amorphous and crystal structures but also among metastable crystal polymorphs This dissertation summarizes work which encompasses research spanning molecular models and inorganic crystallization with added commentary on outreach and communication

Stability Limits and Structure of Glasses, Liquids, and Crystals from Computer Simulation Mahin Hemmati,1996

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